CLAIMS

What we claim is:

5 1. A method of characterizing electrochemical cell components, comprising:

preparing a sample of an electrode material in contact with an electrolyte;

obtaining self-heating data, power-temperature data or power-time data for the sample using a calorimetry technique; and

10 developing a power function for the sample using the self-heating, power-temperature or power-time data, the power function representative of thermal power per unit mass of the sample as a function of temperature and amount of reactant remaining from a reaction of the electrode material and electrolyte of the sample.

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2. The method of claim 1, wherein preparing the sample comprises preparing the sample using less than about 100 grams of the electrode material.

3. The method of claim 1, wherein preparing the sample comprises

20 preparing the sample using between about 1 and about 10 grams of the electrode material.

4. The method of claim 1, wherein preparing the sample comprises preparing the sample using between about 1 milligram and about 1 gram of the

25 electrode material.

5. The method of claim 1, wherein the electrode material comprises cathode material.

30 6. The method of claim 1, wherein the electrode material comprises anode material.

7.   The method of claim 1, wherein the electrode material comprises lithium.

8.   The method of claim 1, wherein obtaining the self-heating data comprises

5   obtaining temperature versus time data of the sample during reaction under

substantially adiabatic conditions.

9.   The method of claim 1, wherein using the calorimetry technique

comprises using an accelerating rate calorimetry technique.

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10.   The method of claim 1, wherein using the calorimetry technique

comprises using a differential scanning calorimetry technique.

11.   A method of characterizing electrochemical cell components,

15   comprising:

preparing a first sample of a cathode material in contact with an

electrolyte;

preparing a second sample of an anode material in contact with the

electrolyte;

20   obtaining first and second self-heating, power-temperature or power-time

data for the first and second samples, respectively, using a calorimetry

technique; and

developing a first power function for the first sample and a second power

function for the second sample using the first and second self-heating, power-

25   temperature or power-time data, respectively, the first power function

characterizing a reaction between the cathode material and the electrolyte in

terms of thermal power per unit mass of the cathode sample material, and the

second power function characterizing a reaction between the anode material and

the electrolyte in terms of thermal power per unit mass of the anode sample

30   material.

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12.   The method of claim 11, wherein preparing the first sample comprises preparing the first sample using less than about 100 grams of the cathode material and preparing the second sample comprises preparing the second sample using less than about 100 grams of the anode material.

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13.   The method of claim 11, wherein preparing the first sample comprises preparing the first sample using between about 1 and about 10 grams of the cathode material and preparing the second sample comprises preparing the second sample using between about 1 and about 10 grams of the anode material.

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14.   The method of claim 11, wherein preparing the first sample comprises preparing the first sample using between about 1 milligram and about 1 gram of the cathode material and preparing the second sample comprises preparing the second sample using between about 1milligram and about 1 gram of the anode

15   material.

15.   The method of claim 11, wherein the cathode and anode material each comprises lithium.

20   16.   The method of claim 11, wherein obtaining the first and second self-heating data comprises obtaining temperature versus time data of the first and second samples during reaction under substantially adiabatic conditions, respectively.

25   17.   The method of claim 11, wherein using the calorimetry technique comprises using an accelerating rate calorimetry technique.

18.   The method of claim 11, wherein using the calorimetry technique comprises using a differential scanning calorimetry technique.

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19. A method of characterizing an electrochemical cell, comprising:

defining one or more physical parameters of the electrochemical cell;

providing a first power function characterizing a reaction between a
cathode and an electrolyte in terms of thermal power per unit mass of cathode

5   material;

providing a second power function characterizing a reaction between an
anode and the electrolyte in terms of thermal power per unit mass of anode
material; and

predicting, using the first and second power functions and the physical

10   parameters of the electrochemical cell, a response of the cell to a specified
operating condition.

20. The method of claim 19, wherein the method is implemented using a
computer and user-interface coupled to the computer.

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21. The method of claim 19, wherein:

defining one or more physical parameters of the cell further comprises
adjusting the physical parameters of the cell; and

predicting the response of the cell further comprises predicting the

20   response of the cell using the first and second power functions and the adjusted
physical parameters of the cell.

22. The method of claim 19, wherein defining one or more physical
parameters of the cell further comprises receiving user input data representative

25   of physical parameters of the cell.

23. The method of claim 22, wherein receiving user input data further
comprises:

presenting to a user an input field corresponding to each physical

30   parameter of the cell; and

receiving input data from the user in each of the input fields.

24. The method of claim 19, wherein defining one or more physical parameters of the cell further comprises receiving physical parameters of the cell electronically.

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25. The method of claim 19, wherein defining one or more physical parameters of the cell further comprises receiving physical parameters of the cell from an external host processor.

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26. The method of claim 19, wherein defining one or more physical parameters of the cell further comprises defining one or more physical parameters for each of an anode and a cathode of the cell.

27. The method of claim 26, further wherein:

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defining physical parameters for each of the anode and cathode of the cell further comprises adjusting the physical parameters of one or both of the anode and cathode; and

predicting the response of the cell further comprises predicting the response of the cell using the first and second power functions and the adjusted

20 physical parameters of one or both of the anode and cathode.

28. The method of claim 19, wherein the specified operating condition comprises a condition of constant or varying ambient temperature.

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29. The method of claim 19, wherein the specified operating condition comprises a condition of a constant or varying current applied to the cell.

30. The method of claim 19, wherein the specified operating condition comprises a condition of an external short-circuit connected to the cell.

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31.   The method of claim 19, wherein the specified operating condition comprises a condition of a short-circuit internal to the cell.

32.   A system for characterizing an electrochemical cell, comprising:

5   a processor;

a user-interface, coupled to the processor, comprising an input device operable by a user for entering one or more physical parameters of the electrochemical cell; and

memory, coupled to the processor, that stores a cathode power function

10   characterizing a reaction between a cathode and an electrolyte in terms of thermal power per unit mass of cathode material and further stores an anode power function characterizing a reaction between an anode and the electrolyte in terms of thermal power per unit mass of anode material, the processor computing a response of an electrochemical cell to a specified operating condition using the

15   cathode and anode power functions and the physical parameters of the electrochemical cell.

33.   The system of claim 32, wherein:

the input device is operable by the user to enter physical parameters of an

20   anode and a cathode of the cell; and

the processor computes the response of the electrochemical cell to the specified operating condition using the cathode and anode power functions and the entered physical parameters of the anode and cathode of the electrochemical cell.

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34.   The system of claim 32, wherein:

the input device is operable by the user to adjust physical parameters of the cell; and

the processor computes the response of the electrochemical cell to the

30   specified operating condition using the cathode and anode power functions and the adjusted physical parameters of the electrochemical cell.

35.   The system of claim 32, wherein:

the input device is operable by the user to adjust physical parameters of an anode and a cathode of the cell; and

the processor computes the response of the electrochemical cell to the specified operating condition using the cathode and anode power functions and the adjusted physical parameters of the anode and cathode of the electrochemical cell.

36.   The system of claim 32, wherein the user-interface comprises a display, and the input device is operable by the user for entering physical parameters of the electrochemical cell into input fields presented on the display.

37.   The system of claim 32, wherein the user-interface comprises a display, and the input device is operable by the user for entering physical parameters of an anode and a cathode of the electrochemical cell into input fields presented on the display.

38.   The system of claim 32, wherein the memory that stores the anode and cathode power functions is partially or completely situated remotely from the processor.

39.   The system of claim 32, further comprising a calorimeter system coupled to the processor.

40.   The system of claim 32, wherein the calorimeter system comprises an accelerating rate calorimeter or a differential scanning calorimeter.

41. A method of characterizing electrochemical cell components, comprising:

defining one or more physical parameters of an electrochemical cell;

characterizing a reaction between a cathode and an electrolyte in terms of

5 thermal power per unit mass of cathode material by defining a first power function;

characterizing a reaction between an anode and the electrolyte in terms of thermal power per unit mass of anode material by defining a second power function; and

10 predicting, using the first and second power functions and the physical parameters of the electrochemical cell, a response of the cell to a specified operating condition.

42. The method of claim 41, wherein characterizing the respective

15 cathode/electrolyte and anode/electrolyte reactions comprises modeling the respective reactions assuming an autocatalytic reaction mechanism.

43. The method of claim 41, wherein the first power function, P_c, associated with the cathode/electrolyte reaction is given by the following equations:

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$$\frac{du}{dt} = k(1 - u)(\beta + u^{0.5})$$

$$\frac{dT}{dt} = \frac{h}{C'_{tot}} * \frac{du}{dt}$$

25 $$P_c = H \, du/dt$$

where, u represents a dimensionless fractional degree of conversion, k represents a reaction rate constant defined by $k = \gamma \exp(-E_a/k_b T)$, γ represents a frequency factor expressed in terms of minutes^{-1}, E_a represents activation energy, k_b

represents Boltzmann's constant, T represents a temperature of the cell, β represents a dimensionless parameter of autocatalysis, h represents total heat which can be evolved by a sample of cathode material during reaction expressed in terms of Joules, C'_{tot} represents a total heat capacity of the reactant and a sample calorimeter bomb expressed in terms of J/K, and H represent total heat generated by the cathode/electrolyte reaction per gram of cathode material.

44.   The method of claim 41, wherein the second power function, P_a, associated with the anode/electrolyte reaction is given by:

$$P_a = H_2 \mid \frac{dx_2}{dt} \mid + H_1 \mid \frac{dx_1}{dt} \mid$$

where,

$$\frac{dx_2}{dt} = -\gamma_2 \exp^{-E_2/k_bT} x_2^{0.5}$$

$$\frac{dx_1}{dt} = -\gamma_1 \exp^{-E_1/k_bT} x_1 \exp^{-((x_{3o}+x_{2o})+f(x_{1o}-x_1))/(x_{3o}+x_{2o})}$$

and

$$\frac{dx_3}{dt} = -\frac{dx_1}{dt} - \frac{dx_2}{dt}$$

further where, x_1 represents an amount of type 1 lithium measured as x in Li_xC_6, x_2 is an amount of type 2 lithium, measured per six carbons, and x_3 is an amount of type 3 lithium, measured per six carbons, x_{1o}, x_{2o}, and x_{3o} are initial amounts of lithium after electrochemical discharge and before heating, E_1 and E_2 are activation energies, and γ_1 and γ_2 are frequency factors, f is a constant of

proportionality that governs how fast the layer of reaction products on the surface of the carbon grows as type 1 lithium is converted to type 3 lithium, and H_1 and H_2 are the heat per gram of carbon due to the changes $\Delta x_1 = -1$ and $\Delta x_2 = -1$, respectively.

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45. The method of claim 41, wherein:

characterizing the cathode/electrolyte reaction comprises characterizing the cathode/electrolyte reaction using less than about 100 grams of cathode material; and

10 characterizing the anode/electrolyte reaction comprises characterizing the anode/electrolyte reaction using less than about 100 grams of anode material.

46. The method of claim 41, wherein:

characterizing the cathode/electrolyte reaction comprises characterizing 15 the cathode/electrolyte reaction using between about 1 and about 10 grams of cathode material; and

characterizing the anode/electrolyte reaction comprises characterizing the anode/electrolyte reaction using between about 1 and about 10 grams of anode material.

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47. The method of claim 41, wherein:

characterizing the cathode/electrolyte reaction comprises characterizing the cathode/electrolyte reaction using between about 1 milligram and about 1 gram of cathode material; and

25 characterizing the anode/electrolyte reaction comprises characterizing the anode/electrolyte reaction using between about 1 milligram and about 1 gram of anode material.

48. The method of claim 41, wherein the cathode and anode material each 30 comprises lithium.

49.   The method of claim 41, wherein characterizing the first and second power functions comprises obtaining temperature versus time data of each of the cathode/electrolyte and anode/electrolyte reactions.

5   50.   The method of claim 41, wherein characterizing the first and second power functions comprises using a calorimetry technique.

51.   The method of claim 50, wherein using the calorimetry technique comprises using an accelerating rate calorimetry technique or a differential
10   scanning calorimetry technique.

52.   The method of claim 41, wherein the specified operating condition comprises a condition of constant or varying ambient temperature.

15   53.   The method of claim 41, wherein the specified operating condition comprises a condition of a constant or varying current applied to the cell.

54.   The method of claim 41, wherein the specified operating condition comprises a condition of an external short-circuit connected to the cell.
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55.   The method of claim 41, wherein the specified operating condition comprises a condition of a short-circuit internal to the cell.

56.   A computer readable medium embodying program instructions for
25   characterizing electrochemical cell components, comprising:
        characterizing a reaction between a cathode and an electrolyte in terms of thermal power per unit mass of cathode material by defining a first power function;
        characterizing a reaction between an anode and the electrolyte in terms of
30   thermal power per unit mass of anode material by defining a second power function;

defining one or more physical parameters of the electrochemical cell; and predicting, using the first and second power functions and the physical parameters of the electrochemical cell, a response of the cell to a specified operating condition.

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57.   The medium of claim 56, wherein characterizing the respective cathode/electrolyte and anode/electrolyte reactions comprises modeling the respective reactions assuming an autocatalytic reaction mechanism.

10   58.   The method of claim 56, wherein the first power function, P_c, associated with the cathode/electrolyte reaction is given by the following equations:
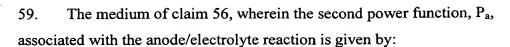
$$\frac{du}{dt} = k(1-u)(\beta + u^{0.5})$$

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$$\frac{dT}{dt} = \frac{h}{C'_{tot}} * \frac{du}{dt}$$

$$P_c = H \, du/dt$$

where, u represents a dimensionless fractional degree of conversion, k represents
20   a reaction rate constant defined by $k = \gamma \exp(-E_a/k_b T)$, γ represents a frequency factor expressed in terms of minutes^{-1}, E_a represents activation energy, k_b represents Boltzmann's constant, T represents a temperature of the cell, β represents a dimensionless parameter of autocatalysis, h represents total heat which can be evolved by a sample of cathode material during reaction expressed
25   in terms of Joules, C'_{tot} represents a total heat capacity of the reactant and a sample calorimeter bomb expressed in terms of J/K, and H represent total heat generated by the cathode/electrolyte reaction per gram of cathode material.

59.   The medium of claim 56, wherein the second power function, P_a, associated with the anode/electrolyte reaction is given by:

$$P_a = H_2 \mid \frac{dx_2}{dt} \mid + H_1 \mid \frac{dx_1}{dt} \mid$$

5   where,

$$\frac{dx_2}{dt} = -\gamma_2 \exp^{-E_2/k_bT} x_2^{0.5}$$

$$\frac{dx_1}{dt} = -\gamma_1 \exp^{-E_1/k_bT} x_1 \exp^{-((x_{3o}+x_{2o})+f(x_{1o}-x_1))/(x_{3o}+x_{2o})}$$

and

$$\frac{dx_3}{dt} = -\frac{dx_1}{dt} - \frac{dx_2}{dt}$$

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further where, x_1 represents an amount of type 1 lithium measured as x in Li_xC_6, x_2 is an amount of type 2 lithium, measured per six carbons, and x_3 is an amount of type 3 lithium, measured per six carbons, x_{1o}, x_{2o}, and x_{3o} are initial amounts of lithium after electrochemical discharge and before heating, E_1 and E_2 are

15   activation energies, and γ_1 and γ_2 are frequency factors, f is a constant of proportionality that governs how fast the layer of reaction products on the surface of the carbon grows as type 1 lithium is converted to type 3 lithium, and H_1 and H_2 are the heat per gram of carbon due to the changes $\Delta x_1 = -1$ and $\Delta x_2 = -1$, respectively.

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60.   The medium of claim 56, wherein:

defining one or more physical parameters of the cell further comprises adjusting the physical parameters of the cell; and

predicting the response of the cell further comprises predicting the response of the cell using the first and second power functions and the adjusted physical parameters of the cell.

5   61.   The medium of claim 56, wherein defining one or more physical parameters of the cell further comprises receiving user input data representative of physical parameters of the cell.

62.   The medium of claim 61, wherein receiving user input data further

10   comprises:

     presenting to a user an input field corresponding to each physical parameter of the cell; and

     receiving input data from the user in each of the input fields.

15   63.   The medium of claim 56, wherein defining one or more physical parameters of the cell further comprises receiving physical parameters of the cell electronically.

64.   The medium of claim 56, wherein defining one or more physical

20   parameters of the cell further comprises defining one or more physical parameters for each of an anode and a cathode of the cell.

65.   The medium of claim 64, further wherein:

     defining physical parameters for each of the anode and cathode of the

25   cell further comprises adjusting the physical parameters of one or both of the anode and cathode; and

     predicting the response of the cell further comprises predicting the response of the cell using the first and second power functions and the adjusted physical parameters of one or both of the anode and cathode.

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66.   The medium of claim 56, wherein the specified operating condition comprises a condition of constant or varying ambient temperature.

67.   The medium of claim 56, wherein the specified operating condition comprises a condition of a constant or varying current applied to the cell.

68.   The medium of claim 56, wherein the specified operating condition comprises a condition of an external short-circuit connected to the cell.

69.   The medium of claim 56, wherein the specified operating condition comprises a condition of a short-circuit internal to the cell.

70.   The medium of claim 56, wherein the medium comprises one or more magnetic data storage diskettes, direct access data storage disks, magnetic tape, alterable or non-alterable electronic read-only memory, flash memory, optical storage devices or signal-bearing media comprising digital, analog, and/or communication links and wireless transmission media or propagated signal media.